

Trifluoromethanesulfonic acid
1493-13-6 | DTXSID2044397

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 171 °C

Global applicability domain: Outside

Local applicability domain index: 2.37e-01

Confidence level: 5.83e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Trifluoromethanesulfonic acid</div> <div>Measured: 166</div> <div>Predicted: 171</div>	<div>Image not found</div> <div>1-Perfluorobutanesulfonic acid</div> <div>Measured: 211</div> <div>Predicted: 212</div>	<div>Image not found</div> <div>Dimethyl phosphate</div> <div>Measured: 174</div> <div>Predicted: 181</div>
<div>Image not found</div> <div>1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5- undecafluoro-</div> <div>Measured: 225</div> <div>Predicted: 223</div>	<div>Image not found</div> <div>Pentanedioic acid</div> <div>Measured: 303</div> <div>Predicted: 310</div>	